## 1,1,1,2-Tetrachloroethane 630-20-6 | DTXSID2021317

## **Model Performance**

Model	Data	

# Weighted KNN model

5-fold CV (75%)		Training (75°	Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.91	1.08	0.91	1.08	0.92	1.00	

#### Model Results

Predicted value: 20.2 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.08e-01

Confidence level: 6.82e-01

## Nearest Neighbors from the Training Set

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Pentatriacontane Measured: 12.0 Predicted: 8.42e-12

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2,3-Dimethylbutane Measured: 4.62 Predicted: 313

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Cyclohexane Measured: 89.0 Predicted: 91.3

#### Image not found

Thiabendazole Measured: 458 Predicted: 7.68e-07

#### Image not found

Ethyl acetoacetate

Measured: 380

Predicted: 6.86e-01